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H^1-SECOND ORDER CONVERGENT ESTIMATES FOR NON FICKIAN MODELS

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ABSTRACT: In this paper we study numerical methods for integro-differential initial boundary value problems that arise, naturally, in many applications such as heat conduction in materials with memory, diffusion in polymers and diffusion in porous media. We propose finite difference methods to compute approximations for the continuous solutions of such problems. For those methods we analyze the stability and study the convergence. We prove a supraconvergent estimate. As such methods can be seen as lumped mass methods, our supraconvergent result is a superconvergent result in the context of finite element methods. Numerical results illustrating the theoretical results are included.

KEYWORDS: Non Fickian models, Finite difference method, Piecewise linear finite element method, Supraconvergence, Superconvergence.

1. Introduction

We consider the semi-discretization of the integro-differential equation

$$\frac{\partial u}{\partial t}(t) + Au(t) = \int_0^t B(s,t)u(s)\,ds + f(t), t \in (0,T], \tag{1}$$

where $u(t)$ denotes a function defined on $[a,b]$ when $t \in [0,T]$ is fixed, A and $B(s,t)$ represent the following operators

$$Au(x,t) = -\frac{\partial}{\partial x}(a_2(x)\frac{\partial u}{\partial x}(x,t)) + \frac{\partial}{\partial x}(a_1(x)u(x,t)) + a_0(x)u(x,t),$$

$$B(s,t)u(x,t) = -\frac{\partial}{\partial x}(b_2(s,t,x)\frac{\partial u}{\partial x}(x,t)) + \frac{\partial}{\partial x}(b_1(s,t,x)u(x,t))$$
$$+b_0(s,t,x)u(x,t),$$

for $x \in (a,b)$, $s,t \in (0,T]$. We assume that (1) is complemented with homogeneous boundary conditions and an initial condition $u(x,0) = u_0(x)$, $x \in [a,b]$. For the coefficient functions we assume some smoothness that will be specified later.

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Integro-differential equations of type (1) arise in several applications as for instance transport in heterogeneous media ([7], [19], [28]) and heat propagation in materials with memory ([21]).

Transport in media or heat propagation phenomena are traditionally modeled by the convection-diffusion equation

$$\frac{\partial u}{\partial t} + \nabla J = f, \tag{2}$$

where u denotes the concentration, J represents the mass flux and f denotes the reaction term. In (2) J can be expressed as

$$J = J_{adv} + J_{dif} + J_{dis}, \tag{3}$$

where

$$J_{adv} = vu \tag{4}$$

represents the advection mass due to the the fluid velocity v,

$$J_{dif} = -D_m \nabla u \tag{5}$$

denotes the mass flux due to molecular diffusion, being D_m the effective molecular diffusion coefficient, and J_{dis} satisfies the so called Fick's law

$$J_{dis} = -D_d \nabla u$$

and represents the dispersive mass flux associated with random deviations of fluid velocities within the porous space from their macroscopic value v. In the definition of J_{dis}, D_d denotes the dispersive tensor.

Combining (2) with (3) we obtain the parabolic equation

$$\frac{\partial u}{\partial t} + \nabla(vu) = \nabla((D_m I + D_d)\nabla u) + f, \tag{6}$$

where I is the identity tensor.

Equation (6) gives good accurate results in laboratory environment for perfectly homogeneous media. Nevertheless when non homogeneous media are considered, deviations of the Fickian behavior are observed. In this case the main sources for such deviations are the small-scale and large-scale heterogeneities ([19], [28]). From the theoretical point of view, as the equation (6) is of parabolic type, it induces infinite propagation speed.

In order to circumvent the pathologic behavior of the convection-diffusion-reaction (6) several approaches were proposed in the literature. The reference [28] summarizes some of them. The approach that leads to a simplified version of equation (1) is to consider that the dispersive mass flux satisfies the following differential equation

$$\tau \frac{\partial J_{dis}}{\partial t}(x,t) + J_{dis}(x,t) = -D_d \nabla u(x,t), \tag{7}$$

where τ is a delay parameter ([26]). We remark that the left hand side of (7) is a first order approximation of the left hand side of

$$J_{dis}(x, t+\tau) = -D_d \nabla u(x,t),$$

which means that the dispersion mass flux at the point x at the time $t+\tau$ depends on the gradient of the concentration at the same point but at a delayed time.

From (2) to (7) and considering non reactive flows, we obtain the hyperbolic equation

$$\frac{\partial^2 u}{\partial t^2} + \nabla \frac{\partial}{\partial t}(vu) + \frac{1}{\tau}\frac{\partial u}{\partial t} + \frac{1}{\tau}\nabla(vu) = \frac{\partial}{\partial t}\nabla(D_m \nabla u) + \frac{1}{\tau}\nabla(D_m \nabla u) + \frac{1}{\tau}\nabla(D_d \nabla u). \tag{8}$$

To avoid the mixed derivatives that arise in the equation (8) we point out that (7) leads to

$$J_{dis}(t) = -\frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} D_d \nabla u(s)\, ds, \tag{9}$$

provided that $J_{dis}(0) = 0$. Combining the partition (3), where J_{adv}, J_{dif} and J_{dis} are given by (4), (5) and (9), respectively, with (2) we obtain the integro-differential equation

$$\frac{\partial u}{\partial t} + \nabla(vu) - \nabla(D_m \nabla u) = \frac{1}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} \nabla(D_d \nabla u)(s)\, ds + f. \tag{10}$$

This equation is an example of the integro-differential equation (1).

Initial boundary value problems defined with integro-differential equations of type (1) have been studied numerically. We mention without being exhaustive [24], [25], [32], [35] for the study of the semi-discrete approximations for the solution when finite element method is considered. Generally, in those papers, it is shown that several results known for the semi-discrete approximations for the solution of Fickian parabolic problems also hold for the semi-discrete approximation for the solution of (1). For instance, it is established for the two dimensional version of (1) that, under convenient assumptions on the partition of the domain, the semi-discrete approximation defined using piecewise linear finite element method is second order convergent with respect to the L^2-norm and it is first order convergent with respect to the H^1-norm. This results was also considered in [29] for a semi-discrete lumped mass approximation but with respect to discrete norms and assuming that the solution of the continuous problems are smooth enough (initial condition in H^3).

Second order estimates for the semi-discrete approximation with respect to the L^2-norm were obtained for finite volume approximations in [10] and [11] provided that the exact solution is in H^3. The previous smoothness assumption was weakened in [30] where second order estimates were also obtained if the solution is in H^2.

Integro-differential problems defined by equation (1) can be rewritten as equivalent systems composed by a partial differential equation involving only a time derivative and an integro-differential equation involving only partial derivatives with respect to the space variables and the integral term. This approach was used for instance in [12] where mixed finite element methods were studied.

Finite difference methods (FDM) for initial boundary value problems (IBVP) defined by (1) were considered by the authors recently in [1], [5], [6] and [16], where schemes presenting the same qualitative behaviour of the correspondent continuous models with respect to stability were proposed. In [16], for $a_2 = a_1 = a_0 = 0, b_1 = b_0 = 0$ and $b_2(s,t,x) = \dfrac{\beta}{\tau} e^{-\frac{s-t}{\tau}}$, it was shown that the character of (1) is related with both parabolic and hyperbolic type.

Application of integro-differential models on drug release were considered in [3], [4] and [16].

The aim of this paper is to study a semi-discretization for the IBVP (1) with homogeneous Dirichlet boundary conditions. The method that we propose can be obtained combining a piecewise linear finite element semi-discretization with a quadrature rule in space. This method can be seen as a lumped mass method. The stability and convergence analysis of the semi-discrete solution will be presented. Concerning the error estimates, we establish a second order convergence estimate with respect to the H^1-norm. This result shows that our method presents a supraconvergent behavior, that is, the convergence order is greater than the order of the truncation error. Supraconvergent finite difference schemes have been considered in the literature for elliptic equations and for parabolic equations. Without being exhaustive we point out [2], [8], [9], [13], [14], [17], [18], [20], [22], [23] and [27]. Here we prove that the L^2-norm of the gradient of the error is second order convergent, being this property known as supercloseness of the gradient ([33]). The results obtained in [2] have a central role in the proof of the convergence result. The paper is organized as follows. In Section 2 we introduce the method, de basic definitions and the notation used. Section 3 focuses on the stability analysis of the semi-discrete solution. The convergence analysis is presented in Section 4. In Section 5 we illustrate the second convergence order of our method with some numerical results. Finally, in Section 6, we present the conclusions.

2. A fully semi-discrete Galerkin approximation

We start with the Galerkin formulation of our IBVP and its discretization by linear finite element with quadrature. By $H_0^r(a,b)$, $r \in \mathbb{N}_0$, we represent the usual Sobolev spaces where we consider the usual norms $\|.\|_r$, $r \in \mathbb{N}_0$. For $r = 0$ we use the notation $H_0^0(a,b) = L^2(a,b)$ were we consider the usual inner product $(.,.)_0$. By $L^2(0,T,H_0^r(a,b))$ we represent the space of functions v defined on $[a,b]\times[0,T]$, such that $v(t)$, which denotes the function v when t is fixed, is in $H_0^r(a,b)$ and

$$\int_0^T \|v(t)\|_r^2\, dt \tag{11}$$

is finite.

We consider the following variational formulation of our problem:

$$\text{find } u \in L^2(0,T,H_0^1(a,b)) \text{ such that } \frac{\partial u}{\partial t}(t) \in L^2(a,b) \text{ and}$$
$$\begin{cases} (\dfrac{\partial u}{\partial t}(t), v)_0 + a(u(t),v) = \displaystyle\int_0^t b(s,t,u(s),v)\, ds + (f(t),v)_0,\ t \in (0,T], \\ \hfill \text{for all } v \in H_0^1(a,b), \\ u(0) = u_0, \end{cases} \tag{12}$$

where $a(.,.)$ and $b(s,t,.,.)$ are the bilinear forms defined by

$$a(v,w) = (a_2 v', w')_0 - (a_1 v, w')_0 + (a_0 v, w)_0, \tag{13}$$

for $v, w \in H_0^1(a,b)$, and

$$b(s,t,v,w) = (b_2(s,t)v', w')_0 - (b_1(s,t)v, w')_0 + (b_0(s,t)v, w)_0, \tag{14}$$

for $v, w \in H_0^1(a,b)$.
The coefficient function of the integro-differential equation (1) are assumed to be smooth enough, e.g, $a_2, b_2(s,t) \in C[a,b], a_0, a_1, b_0(s,t), b_1(s,t) \in W^{2,\infty}(a,b)$, for $s, t \in (0,T]$.

The discretization of (12) is obtained in the following way. We first introduce in $[a,b]$ the grid

$$\mathbb{I}_h := \{a = x_0 < x_1 < \cdots < x_{N-1} < x_N = b\},$$

where h is the vector of mesh-sizes $h_j = x_j - x_{j-1}, j = 1, \ldots, N$. By $W_{h,0} := \{u_h, v_h, w_h, \ldots\}$ we denote the space of real-valued grid functions defined on $\mathbb{I}_h$ null on the boundary points. In $W_{h,0}$ we introduce the inner product

$$(v_h, w_h)_h = \sum_{i=1}^{N-1} h_{i+1/2} v_h(x_i) w_h(x_i), \text{ for } v_h, w_h \in W_{h,0}, \tag{15}$$

where $h_{i+1/2} = (h_i + h_{i+1})/2$. The norm induced by the inner product (15) is denoted by $\|.\|_h$

Let R_h denote the operator of pointwise restriction to the grid $\mathbb{I}_h$. We now introduce the discretization of the bilinear forms $a(.,.)$ and $b(s,t,.,.)$. By $a_h(.,.)$ and $b_h(s,t,.,.)$ we represent the following bilinear forms

$$\begin{aligned} a_h(v_h, w_h) = (M(a_2)(P_h v_h)', (P_h w_h)')_0 - (M(P_h(R_h a_1 v_h)), (P_h w_h)')_0 \\ +(R_h a_0 v_h, w_h)_h, \end{aligned} \tag{16}$$

for $v_h, w_h \in W_{h,0}$, and

$$\begin{aligned} b_h(s,t,v_h,w_h) &= (M(b_2(s,t))(P_h v_h)', (P_h w_h)')_0 \\ &-(M(P_h(R_h b_1(s,t) v_h)), (P_h w_h)')_0 \\ &+(R_h b_0(s,t) v_h, w_h)_h, \end{aligned} \tag{17}$$

for $v_h, w_h \in W_{h,0}$. In (16) and (17) we use the notation $M(q)(x) = q(x_{i+1/2})$ for $x \in [x_i, x_{i+1}], i = 0, \ldots, N-1$.

We assume that $a_h(.,.)$ is continuous

$$|a_h(v_h, w_h)| \leq \alpha_c \|P_h v_h\|_1 \|P_h w_h\|_1, \text{ for all } v_h, w_h \in W_{h,0},$$

and elliptic in the sense that

$$a_h(v_h, v_h) \geq \alpha_0 \|P_h v_h\|_1^2, \text{ for all } v_h \in W_{h,0}. \tag{18}$$

We also suppose that $b_h(s,t,.,.)$ is uniformly bounded, that is,

$$|b_h(s,t,v_h,w_h)| \leq \beta_0 \|P_h v_h\|_1 \|P_h w_h\|_1, \text{for all } v_h, w_h \in W_{h,0},\ s,t \in [0,T]. \tag{19}$$

Remark 1. *The bilinear form $a_h(.,.)$ satisfies the assumption (18) provided that $a_2, a_0 \geq \gamma_0 > 0$ in $[a,b]$, and*

$$\gamma_0 - \frac{1}{4\eta^2}\|a_1\|_\infty^2 \geq 0 \tag{20}$$

or

$$\gamma_0\Big(\frac{1}{3(b-a)^2} + 1\Big) - \Big(\frac{\eta^2}{3(b-a)^2} + \frac{1}{4\eta^2}\|a_1\|_\infty^2\Big) \geq 0, \tag{21}$$

for η such that

$$\gamma_0 - \eta^2 > 0. \tag{22}$$

In fact, as for $a_h(.,.)$ we have

$$a_h(v_h, v_h) \geq (\gamma_0 - \eta^2)\|(P_h v_h)'\|^2 + \Big(\gamma_0 - \frac{1}{4_\eta^2}\|a_1\|_\infty^2\Big)\|v_h\|_h^2,$$

using the Friedrich-Poincaré inequality and $\|P_h v_h\|^2 \geq \dfrac{1}{3}\|v_h\|_h^2$, we immediately conclude the assumption (18) under the assumptions (20) or (21), for η satisfying (22).

If the coefficient functions of $b_h(s,t,.,.)$ are bounded then this bilinear form satisfies (19).

Let g be a function defined on $[a,b]$. We denote by $(g)_h$ the grid function

$$(g)_h(x_i) = \frac{1}{h_{i+1/2}}\int_{x_{i-1/2}}^{x_{i+1/2}} g(x)\,dx, i = 1,\dots,N-1, \tag{23}$$

$(g)_h(x_0) = (g)_h(x_N) = 0$, where $x_{i+1/2} = x_i + \dfrac{h_{i+1}}{2}, x_{i-1/2} = x_i - \dfrac{h_i}{2}$.

The semi-discrete variational problem has the form:

$$\text{find } u_h(t) \in W_{h,0} \text{ such that}$$
$$\begin{cases} (\frac{du_h}{dt}(t), v_h)_h + a_h(u_h(t), v_h) = \int_0^t b_h(s,t,u_h(s),v_h)\,ds \\ \qquad\qquad +((f(t))_h, v_h)_h,\ t \in (0,T], \text{for all}\, v_h \in W_{h,0}, \\ u_h(0) = u_{0,h}, \end{cases} \tag{24}$$

where $u_{0,h} \in W_{h,0}$ is an approximation of u_0.

The semi-discrete variational problem (24) is equivalent to a standard finite semi-discretization of (1) on nonuniform grids which we derive in what follows. We use the divided differences

$$(D_c v_h)(x_i) = \frac{v_h(x_{i+1}) - v_h(x_{i-1})}{x_{i+1} - x_{i-1}},\ (Dv_h)(x_i) = \frac{v_h(x_{i+1/2}) - v_h(x_{i-1/2})}{x_{i+1/2} - x_{i-1/2}}$$

and

$$(Dv_h)(x_{i+1/2}) = \frac{v_h(x_{i+1}) - v_h(x_i)}{x_{i+1} - x_i},$$

where $v_h(x_{i+1/2})$ is used as far as it makes sense.

Now choosing $v_h \in W_{h,0}$ to vanish in all but one grid point in $\mathbb{I}_h \setminus \{a,\, b\}$ and collecting the terms arising in (24), we obtain for $u_h(t)$ the following ordinary differential problem

$$\begin{cases} \frac{du_h}{dt}(t) + A_h u_h(t) = \int_0^t B_h(s,t) u_h(s)\,ds + (f(t))_h \text{ in } \mathbb{I}_h \setminus \{a,\, b\},\ t \in (0,T], \\ u_h(x_0,t) = u_h(x_N,t) = 0, t \in (0,T], \\ u_h(0) = u_{0,h}, \end{cases} \tag{25}$$

where

$$A_h v_h = -D(a_2 D v_h) + D_c(a_1 v_h) + a_0 v_h$$

and

$$B_h(s,t) v_h = -D(b_2(s,t) D v_h) + D_c(b_1(s,t) v_h) + b_0(s,t) v_h.$$

We remark that $P_h u_h(t)$ is an approximation for the weak solution defined by (12), being $u_h(t)$ the finite difference solution defined by (25).

3. The stability analysis

In what follows we establish the stability of the solution $u_h(t)$ defined by (25) with respect to perturbations of the initial condition $u_{0,h}$.

Theorem 1. *Let us suppose that $a_h(.,.)$ and $b_h(s,t,.,.)$ satisfy (18) and (19) respectively. Then for the solution $u_h(t)$ of (25) holds*

$$\|u_h(t)\|_h^2+\int_0^t \|P_h u_h(s)\|_1^2\,ds \le e^{Ct}C\Big(\|u_h(0)\|_h^2+\int_0^t \|f(s)\|_0^2 e^{-Cs}\,ds\Big),\ t\in[0,T], \tag{26}$$

with

$$C=\frac{\max\{1,\frac{\beta_0^2 T}{2\epsilon^2}\}}{\min\{1,2(\alpha_0-\epsilon^2)\}} \tag{27}$$

for all $\epsilon\neq 0$ such that

$$\alpha_0-\epsilon^2>0. \tag{28}$$

Proof: As $u_h(t)$ satisfies (24) with $v_h=u_h(t)$ we establish

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|u_h(t)\|_h^2+\alpha_0\|P_h u_h(t)\|_1^2 \ &\le \beta_0\int_0^t \|P_h u_h(s)\|_1\|P_h u_h(t)\|_1\,ds\\ &\quad+\frac{1}{2}(\|(f(t))_h\|_h^2+\|u_h(t)\|_h^2).\end{aligned}$$

As we have

$$\int_0^t \|P_h u_h(s)\|_1\|P_h u_h(t)\|_1\,ds\le\frac{1}{4\epsilon^2}\Big(\int_0^t \|P_h u_h(s)\|_1 ds\Big)^2+\epsilon^2\|P_h u_h(t)\|_1^2,$$

for all $\epsilon\neq 0$, we deduce

$$\begin{aligned}\frac{d}{dt}\|u_h(t)\|_h^2+2(\alpha_0-\epsilon^2)\|P_h u_h(t)\|_1^2 \ &\le \frac{\beta_0^2}{2\epsilon^2}\Big(\int_0^t \|P_h u_h(s)\|_1\,ds\Big)^2\\ &\quad+\|(f(t))_h\|_h^2+\|u_h(t)\|_h^2.\end{aligned} \tag{29}$$

Using the inequality

$$\Big(\int_0^t \|P_h u_h(s)\|_1\,ds\Big)^2\le T\int_0^t \|P_h u_h(s)\|_1^2\,ds$$

in (29) and integrating the obtained inequality we get

$$\|u_h(t)\|_h^2 + 2(\alpha_0 - \epsilon^2)\int_0^t \|P_h u_h(s)\|_1^2\,ds \le \int_0^t \|((f(s))_h\|_h^2\,ds + \|u_h(0)\|_h^2 + \frac{\beta_0^2 T}{2\epsilon^2}\int_0^t\int_0^s \|P_h u_h(\mu)\|_1^2\,d\mu\,ds + \int_0^t \|u_h(s)\|_h^2\,ds. \tag{30}$$

Choosing ϵ satisfying (28) we obtain

$$\begin{aligned}\|u_h(t)\|_h^2 + \int_0^t \|P_h u_h(s)\|_1^2\,ds &\le C\Big(\int_0^t \|(f(s))_h\|_h^2\,ds + \|u_h(0)\|_h^2\Big)\\ &\quad + C\int_0^t \Big(\int_0^s \|P_h u_h(\mu)\|_1^2\,d\mu + \|u_h(s)\|_h^2\Big)\,ds\end{aligned} \tag{31}$$

with C defined by (27). Finally considering the Gronwall lemma in (31) we conclude (26).

■

Theorem 2. *Let $u_h(t)$ be the solution of (25) with $a_1 = 0$. If $a_h(.,.)$ satisfies (18), $b_h(s,t,.,.)$ satisfies (19) and*

$$b_h(t,t,v_h,v_h) \ge \beta_e\|P_h v_h\|_1^2, \text{ for all } v_h \in W_{h,0}, \tag{32}$$

and

$$\Big|\frac{\partial b_h}{\partial t}(s,t,v_h,w_h)\Big| \le \beta_d\|P_h v_h\|_1\|P_h w_h\|_1\,, \text{ for all } v_h, w_h \in W_{h,0},\ s,t\in[0,T], \tag{33}$$

then the solution $u_h(t)$ of (25) satisfies

$$\int_0^t \|\frac{du_h}{ds}(s)\|_h^2 ds + \|P_h u_h(t)\|_1^2 + \int_0^t \|P_h u_h(t)\|_1^2 \le e^{Ct}\frac{\max\{1,\alpha_c\}}{\min\{1,\alpha_0-\eta^2, 2\beta_e-\epsilon^2)\}}\Big(\|P_h u_h(0)\|_1^2 + \int_0^t \|f(s)\|^2\,e^{-Cs}\,ds\Big), \tag{34}$$

for $t\in[0,T]$, for ϵ and η such that

$$\alpha_0 - \eta^2 > 0,\ 2\beta_e - \epsilon^2 > 0, \tag{35}$$

with

$$C = \frac{\max\{\frac{\beta_0^2 T}{\eta^2}, \frac{\beta_d^2 T}{2\epsilon^2}\}}{\min\{1,\alpha_0-\eta^2, 2\beta_e-\epsilon^2)\}}\,. \tag{36}$$

Proof: Considering in (24) v_h replaced by $\frac{du_h}{dt}(t)$ we obtain

$$\begin{aligned}\|\frac{du_h}{dt}(t)\|_h^2 + a_h(u_h(t), \frac{du_h}{dt}(t)) &= \int_0^t b_h(s,t,u_h(s), \frac{du_h}{dt}(t))\,ds \\ &+((f(t))_h, \frac{du_h}{dt}(t))_h.\end{aligned} \tag{37}$$

As

$$\frac{d}{dt}a_h(u_h(t),u_h(t)) = 2a_h(u_h(t), \frac{du_h}{dt}(t))$$

and

$$\begin{aligned}\frac{d}{dt}\int_0^t b_h(s,t,u_h(s),u_h(t))\,ds &= b_h(t,t,u_h(t),u_h(t)) \\ &+ \int_0^t b_h(s,t,u_h(s),\frac{du_h}{dt}(t))\,ds \\ &+ \int_0^t \frac{\partial b_h}{\partial t}(s,t,u_h(s),u_h(t))\,ds,\end{aligned}$$

we deduce

$$\begin{aligned}\frac{1}{2}\|\frac{du_h}{dt}(t)\|_h^2 + \frac{1}{2}\frac{d}{dt}a_h(u_h(t),u_h(t)) &\le \frac{d}{dt}\int_0^t b_h(s,t,u_h(s),u_h(t))\,ds \\ &- \int_0^t \frac{\partial b_h}{\partial t}(s,t,u_h(s),u_h(t))\,ds \\ &- b_h(t,t,u_h(t),u_h(t)) + \frac{1}{2}\|(f(t))_h\|_h^2.\end{aligned} \tag{38}$$

Using inequalities (32) and (33) in (38) we establish

$$\begin{aligned}&\frac{1}{2}\|\frac{du_h}{dt}(t)\|_h^2 + \frac{1}{2}\frac{d}{dt}a_h(u_h(t),u_h(t)) + \beta_e\|P_hu_h(t)\|_1 \le \frac{1}{2}\|(f(t))_h\|_h^2 \\ &+ \beta_d\int_0^t \|P_hu_h(s)\|_1\,ds\|P_hu_h(t)\|_1 + \frac{d}{dt}\int_0^t b_h(s,t,u_h(s),u_h(t))\,ds.\end{aligned}$$

Consequently, as

$$\beta_d\int_0^t \|P_hu_h(s)\|_1\,ds\|P_hu_h(t)\|_1 \le \frac{T\beta_d^2}{4\epsilon^2}\int_0^t \|P_hu_h(s)\|_1^2\,ds + \epsilon^2\|P_hu_h(t)\|_1^2$$

holds for any $\epsilon \neq 0$, we have

$$\begin{aligned}\|\frac{du_h}{dt}(t)\|_h^2 + \frac{d}{dt}a_h(u_h(t),u_h(t)) + (2\beta_e - \epsilon^2)\|P_h u_h(t)\|_1^2 \leq \|(f(t))_h\|_h^2 \\ +2\frac{d}{dt}\int_0^t b_h(s,t,u_h(s),u_h(t))\,ds + \frac{\beta_d^2 T}{2\epsilon^2}\int_0^t \|P_h u_h(s)\|_1^2\,ds.\end{aligned} \tag{39}$$

The integration of the inequality (39) leads to

$$\begin{aligned}&\int_0^t \|\frac{du_h}{ds}(s)\|_h^2 ds + a_h(u_h(t),u_h(t)) + (2\beta_e - \epsilon^2)\int_0^t \|P_h u_h(s)\|_1^2\,ds \\ &\quad\leq 2\int_0^t b_h(s,t,u_h(s),u_h(t))\,ds + \frac{\beta_d^2 T}{2\epsilon^2}\int_0^t\int_0^s \|P_h u_h(\mu)\|_1^2\;d\mu\,ds \\ &\quad +a_h(u_h(0),u_h(0)) + \int_0^t \|(f(s))_h\|_h^2\,ds.\end{aligned} \tag{40}$$

Combining (40) with (18) and (19) we deduce

$$\begin{aligned}&\int_0^t \|\frac{du_h}{ds}(s)\|_h^2 ds + (\alpha_0 - \eta^2)\|P_h u_h(t)\|_1^2 + (2\beta_e - \epsilon^2)\int_0^t \|P_h u_h(s)\|_1^2\,ds \\ &\quad\leq \frac{\beta_0^2 T}{\eta^2})\int_0^t \|P_h u_h(s)\|_1^2\,ds + \frac{\beta_d^2 T}{2\epsilon^2}\int_0^t\int_0^s \|P_h u_h(\mu)\|_1^2\;d\mu\,ds \\ &\quad +\alpha_c\|P_h u_h(0)\|_1^2 + \int_0^t \|(f(s))_h\|_h^2\,ds,\end{aligned}$$

and consequently

$$\begin{aligned}&\int_0^t \|\frac{du_h}{ds}(s)\|_h^2 ds + \|P_h u_h(t)\|_1^2 + \int_0^t \|P_h u_h(t)\|_1 \\ &\quad\leq C\int_0^t \big(\int_0^s \|P_h u_h(\mu)\|_1^2\;d\mu + \|P_h u_h(s)\|_1^2\big)ds \\ &\quad +\frac{\max\{1,\alpha_c\}}{\min\{1,\alpha_0-\eta^2,2\beta_e-\epsilon^2\}}\Big(\|P_h u_h(0)\|_1^2 + \int_0^t \|(f(s))_h\|_h^2\,ds\Big)\end{aligned} \tag{41}$$

for ϵ, η satisfying (35) and with C defined by (36).
Applying Grownwall lemma to the inequality (41) we conclude (34).

■

Remark 2. *For $b_h(t,t,.,.)$ holds a remark analogous to Remark 1. Moreover if the coefficient functions of $b_h(s,t,.,.)$ have bounded time derivative then (33) holds and this means that $\dfrac{\partial b_h}{\partial t}(s,t,.,.)$ is bounded.*

4. A supraconvergent estimate

In this section we compute an estimate for the error $P_h e_h(t) = P_h R_h u(t) - P_h u_h(t)$. Following [34] we split the error $P_h e_h(t)$ in the following form

$$\begin{aligned} P_h e_h(t) &= P_h R_h u(t) - P_h \tilde{u}_h(t) + P_h \tilde{u}_h(t) - P_h u_h(t) \\ &=: P_h \rho_h(t) + P_h \theta_h(t) \end{aligned} \tag{42}$$

where $\tilde{u}_h(t)$ is solution of the discrete variational problem

$$a_h(\tilde{u}_h(t), v_h) = (g_h(t), v_h)_h, \text{ for all } v_h \in W_{h,0} \tag{43}$$

with

$$g_h(t) = \int_0^t (B(s,t)u(s))_h - (\frac{\partial u}{\partial t}(t))_h + ((f(t))_h. \tag{44}$$

As we have successively

$$\begin{aligned} \alpha_0 \|P_h \rho_h(t)\|_1^2 &\leq a_h(\rho_h(t), \rho_h(t)) \\ &= a_h(R_h u(t), \rho_h(t)) - (g_h(t), \rho_h(t))_h \\ &= a_h(R_h u(t), \rho_h(t)) - ((Au(t))_h, \rho_h(t))_h \\ &= a_h(R_h u(t), \rho_h(t)) - \sum_{i=1}^{N-1} \int_{x_{i-1/2}}^{x_{i+1/2}} Au(x,t)\, dx \rho_h(x_i,t) \\ &=: \tau_h^{(a)}(\rho_h(t)), \end{aligned}$$

we conclude that

$$\|P_h \rho_h(t))\|_1^2 \leq \frac{1}{\alpha_0} \tau_h^{(a)}(\rho_h(t)). \tag{45}$$

A bound for $P_h \rho_h(t)$ is obtained using Lemma 1 and (45). The proof of this lemma as well the proofs of Lemmas 2, 3 and 4 differ in minor details from the proof of Theorem 3.1 of [2].

Lemma 1. *For the functional* $\tau_h^{(a)}$ *holds the following*

$$|\tau_h^{(a)}(v_h)| \leq C\Big(\sum_{i=1}^{N} h_i^{2r}\|u(t)\|^2_{H^{1+r}(x_{i-1},x_i)}\Big)^{1/2}\|P_h v_h\|_1,\ r\in\{1,2\}, \tag{46}$$

for $v_h \in W_{h,0}$. ■

Proposition 1. *The error* $P_h\rho_h(t)$ *satisfies the estimate*

$$\|P_h\rho_h(t)\|_1 \leq C\Big(\sum_{i=1}^{N} h_i^{2r}\|u(t)\|^2_{H^{1+r}(x_{i-1},x_i)}\Big)^{1/2}, r\in\{1,2\}. \tag{47}$$

■

An estimate for $\|P_h\dfrac{d\rho_h}{dt}(t)\|_1$ can be obtained following the procedure used on the estimation of $\|P_h\rho_h(t)\|_1$. In fact we have successively

$$\begin{aligned}
\alpha_0\|P_h\frac{d\rho_h}{dt}(t)\|_1^2 &\leq a_h(R_h\frac{\partial u}{\partial t}(t)-\frac{d\tilde{u}_h}{dt}(t),\frac{d\rho_h}{dt}(t))\\
&= a_h(R_h\frac{\partial u}{\partial t}(t),\frac{d\rho_h}{dt}(t))-((B(t,t)u(t))_h,\frac{d\rho_h}{dt}(t))_h\\
&\quad -\int_0^t(\frac{\partial}{\partial t}B(s,t)u(s))_h\,ds,\frac{d\rho_h}{dt}(t))_h\\
&\quad +(\frac{\partial^2 u}{\partial t^2}(t))_h+(\frac{\partial f}{\partial t}(t))_h,\frac{d\rho_h}{dt}(t))_h\\
&= a_h(R_h\frac{\partial u}{\partial t}(t),\frac{d\rho_h}{dt}(t))-((A\frac{\partial u}{\partial t}(t))_h,\frac{d\rho_h}{dt}(t))_h\\
&= a_h(R_h\frac{\partial u}{\partial t}(t),\frac{d\rho_h}{dt}(t))-\sum_{i=1}^{N-1}\int_{x_{i-1/2}}^{x_{i+1/2}}A\frac{\partial u}{\partial t}(x,t)\,dx\frac{d\rho_h}{dt}(x_i,t)\\
&=: \tau_h^{(d)}(\frac{d\rho_h}{dt}(t)),
\end{aligned}$$

that is

$$\alpha_0\|P_h\frac{d\rho_h}{dt}(t)\|_1^2 \leq \tau_h^{(d)}(\frac{d\rho_h}{dt}(t)). \tag{48}$$

Lemma 2. *For the functional* $\tau_h^{(d)}$ *holds the following*

$$|\tau_h^{(d)}(v_h)| \leq C\Big(\sum_{i=1}^{N} h_i^{2r}\|\frac{\partial u}{\partial t}(t)\|^2_{H^{1+r}(x_{i-1},x_i)}\Big)^{1/2}\|P_h v_h\|_1,\ r\in\{1,2\}, \tag{49}$$

for $v_h \in W_{h,0}$. ■

From Lemma 2 and the inequality (48) we conclude the next proposition.

Proposition 2. *The error* $P_h\dfrac{d\rho_h}{dt}(t)$ *satisfies the estimate*

$$\|P_h\frac{d\rho_h}{dt}(t)\|_1 \le C\Big(\sum_{i=1}^N h_i^{2r}\|\frac{\partial u}{\partial t}(t)\|^2_{H^{1+r}(x_{i-1},x_i)}\Big)^{1/2}, r\in\{1,2\}. \tag{50}$$

■

Lemma 3. *For the functional* $\tau_h^{(b)}$ *defined by*

$$\tau_h^{(b)}(v_h) = \int_0^t \Big(b_h(s,t,R_hu(s),v_h) - (B(s,t)u(s),v_h)_h\Big)\,ds,$$

for $v_h \in W_{h,0}$, *satisfies*

$$|\tau_h^{(b)}(v_h)| \le C\int_0^t \Big(\sum_{i=1}^N h_i^{2r}\|u(s)\|^2_{H^{1+r}(x_{i-1},x_i)}\Big)^{1/2} ds\,\|P_hv_h\|_1,\ r\in\{1,2\}. \tag{51}$$

■

Lemma 4. *For* $\tau_h^{(u)}(v_h) = (R_h\dfrac{\partial u}{\partial t}(t),v_h)_h - ((\dfrac{\partial u}{\partial t}(t))_h,v_h)_h$, *with* $v_h\in W_{h,0}$, *we have*

$$|\tau_h^{(u)}(v_h)| \le C\Big(\sum_{i=1}^N h_i^{2r}\|\frac{\partial u}{\partial t}(t)\|^2_{H^{1+r}(x_{i-1},x_i)}\Big)^{1/2}\|P_hv_h\|_1,\ r\in\{1,2\}. \tag{52}$$

■

In what follows we use the notation

$$\tau_h^{(b)}(t) = C\int_0^t \Big(\sum_{i=1}^N h_i^{2r}\|u(s)\|^2_{H^{1+r}(x_{i-1},x_i)}\Big)^{1/2} ds$$

and

$$\tau_h^{(u)}(t) = C\Big(\sum_{i=1}^N h_i^{2r}\|\frac{\partial u}{\partial t}(t)\|^2_{H^{1+r}(x_{i-1},x_i)}\Big)^{1/2}.$$

The following lemma has a central role in the main result of this paper.

Lemma 5. *For $P_h\theta_h(t)$ holds the following*

$$\|\theta_h(t)\|_h^2 + 2(\alpha_0 - 3\epsilon^2)\int_0^t \|P_h\theta_h(s)\|_1^2\, ds \leq \frac{\beta_0^2 T}{2\epsilon^2}\int_0^t\int_0^s \|P_h e_h(\mu)\|_1^2\, d\mu\, ds$$
$$+\|\theta(0)\|_h^2 + \frac{1}{2\epsilon^2}\int_0^t \Big(\|\frac{d\rho_h}{ds}(s)\|_h^2 + \tau_h(s)^2\Big)\, ds, \tag{53}$$

for $t \in [0, T]$ and for any $\epsilon \neq 0$.

Proof: It is easy to show that $\dfrac{d\theta_h}{dt}(t)$ is solution of the discrete variational problem

$$(\frac{d\theta_h}{dt}(t), v_h)_h = (\frac{d\tilde{u}_h}{dt}(t), v_h)_h + a_h(u_h(t), v_h) - \int_0^t b_h(s, t, u_h(s), v_h)\, ds$$
$$-((f(t))_h, v_h)_h. \tag{54}$$

Considering in (54) the definition (43) of $\tilde{u}_h(t)$ we obtain

$$(\frac{d\theta_h}{dt}(t), v_h)_h = (\frac{d\tilde{u}}{dt}(t), v_h)_h - a_h(\theta_h(t), v_h) - \int_0^t b_h(s, t, u_h(s), v_h)\, ds$$
$$-((\frac{\partial u}{\partial t}(t))_h, v_h)_h + (\int_0^t (B(s,t)u(s))_h\, ds, v_h)_h$$

which is equivalent to

$$(\frac{d\theta_h}{dt}(t), v_h)_h + a_h(\theta_h(t), v_h) = \int_0^t b_h(s, t, e_h(s), v_h)\, ds$$
$$-(\frac{d\rho_h}{dt}(t), v_h)_h + \tau_h(v_h)\,, \tag{55}$$

for $v_h \in W_{h,0}$ and with $\tau_h(v_h) = \tau_h^{(u)}(v_h) - \tau_h^{(b)}(v_h) := \tau_h(t)\|P_h v_h\|_1$ where $\tau_h(t) = \tau_h^{(u)}(t) - \tau_h^{(b)}(t)$.

Fixing $v_h = \theta_h(t)$ in (55) and using the same kind of arguments that were used in the stability analysis, it can be shown that

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|\theta_h(t)\|_h^2+\alpha_0\|P_h\theta_h(t)\|_1^2 \;\leq\; & \frac{\beta_0^2 T}{4\eta^2}\int_0^t \|P_h e_h(s)\|_1^2\,ds+\eta^2\|P_h\theta_h(t)\|_1^2\\ & +\frac{1}{4\epsilon^2}\|\frac{d\rho_h}{dt}(t)\|_h^2+\epsilon^2\|P_h\theta_h(t)\|_1^2\\ & +\frac{1}{4\sigma^2}\tau_h(t)^2+\sigma^2\|P_h\theta_h(t)\|_1^2,\end{aligned}$$

for $\epsilon \neq 0, \sigma \neq 0$ and for $t \in [0,T]$, which is equivalent to

$$\begin{aligned}\frac{d}{dt}\|\theta_h(t)\|_h^2+2(\alpha_0-3\epsilon^2)\|P_h\theta_h(t)\|_1^2 \;\leq\; & \frac{\beta_0^2 T}{2\epsilon^2}\int_0^t \|P_h e_h(s)\|_1^2\,ds\\ & +\frac{1}{2\epsilon^2}\Big(\|\frac{d\rho_h}{dt}(t)\|_h^2+\tau_h(t)^2\Big),\end{aligned} \tag{56}$$

when $\epsilon = \eta = \sigma$ are considered. Integrating (56) we establish (53).

■

The main theorem is established now.

Theorem 3. *Let u be the solution of the variational problem (12) and $P_h u_h(t)$ its approximation defined by (24). Then, for $t \in [0,T]$, $P_h u_h(t)$ satisfies the error estimate*

$$\begin{aligned}\int_0^t \|P_h e_h(s)\|_1^2\,ds \leq e^{Ct}\Big(&\frac{1}{\alpha_0-3\epsilon^2}\|\theta_h(0)\|_h^2\\ &+\int_0^t e^{-Cs}\Big(\frac{1}{(\alpha_0-3\epsilon^2)\epsilon^2}\Big(\|\frac{d\rho_h}{ds}(s)\|_h^2+\tau_h(s)^2\Big)+2\|P_h\rho_h(s)\|_1^2\Big)\,ds\Big),\end{aligned} \tag{57}$$

where C is defined by

$$C=\frac{\beta_0^2 T}{(\alpha_0-3\epsilon^2)\epsilon^2} \tag{58}$$

and ϵ is such that

$$\alpha_0-3\epsilon^2>0, \tag{59}$$

Proof: The error $P_h e_h$ satisfies the following

$$\int_0^t \|P_h e_h(s)\|_1^2\,ds \leq 2\int_0^t \|P_h\rho_h(s)\|_1^2\,ds+2\int_0^t \|P_h\theta_h(s)\|_1^2\,ds. \tag{60}$$

Using (53) in (60) and choosing ϵ satisfying (59), we obtain

$$\begin{aligned}\int_0^t \|P_h e_h(s)\|_1^2\, ds \ \leq \ & \frac{1}{\alpha_0 - 3\epsilon^2}\Big(\frac{\beta_0^2 T}{\epsilon^2}\int_0^t\int_0^s \|P_h e_h(\mu)\|_1^2\, d\mu\, ds \\ & + \|\theta(0)\|_h^2 + \frac{1}{\epsilon^2}\int_0^t \Big(\|\frac{d\rho_h}{ds}(s)\|_h^2 + \tau_h(s)^2\Big)\, ds\Big) \\ & + 2\int_0^t \|P_h\rho_h(s)\|_1^2\, ds.\end{aligned} \tag{61}$$

Finally the application of the Gronwall lemma to (61) leads to (57).

■

Combining Theorem 3 with Propositions 1, with the definitions of $\tau_h^{(b)}(t)$ and $\tau_h^{(u)}(t)$ we conclude the following result.

Corollary 1. *Let u be the solution of the variational problem (12) and $P_h u_h(t)$ its approximation defined by (24). Then, there exists a positive constant C such that*

$$\begin{aligned}\int_0^t \|P_h e_h(s)\|_1^2\, ds \leq C\Big(&\|P_h u(0) - P_h u_h(0)\|_h^2 \\ & + h_{max}^{2r}\Big(\int_0^t \|u(s)\|_{r+1}^2 ds + \|u(t)\|_{r+1}^2 + \|\frac{\partial u}{\partial t}(t)\|_{r+1}^2\Big)\Big),\end{aligned}$$

for $t \in [0, T]$ and $r \in \{1, 2\}$.

5. Numerical results

In the numerical results that we present in this section, the ordinary differential problem (25) is integrated using the implicit Euler method. We introduce the uniform time grid $\{t_n, n = 0, \ldots, M\}$ with step-size Δt ($M\Delta t = T$) and by u_h^n we represent the numerical solution obtained at time level t_n. The error that we compute in what follows is the maximum of $\|P_h e_h^n\|_1 = \|P_h u(t_n) - P_h u_h^n\|_1$ for n such that $n\Delta t \leq T$, which is denoted by $\|P_h e_h\|_1$.

Example 1. *Let us consider the equation (1) with*

$$\begin{aligned}& a_2(x) = 0.5, a_1(x) = a_0(x) = 0, \\ & b_2(s,t,x) = -\frac{0.5}{\tau} e^{-\frac{t-s}{\tau}}, b_1(s,t,x) = b_0(s,t,x) = 0, \tau = 0.01,\end{aligned} \tag{62}$$

$f = 0$, *and with the conditions*

$$u(0,t) = 1, u(1,t) = 0, t > 0, u(x,0) = 0, x \in [0,1], \tag{63}$$

and $T = 0.1$. *This IBVP can be used to model the diffusion of a substance in the space domain* $[0,1]$ *which is initially empty, with a constant source in the left hand side and the substance that arrives to the right hand side is immediately removed.*

In Figure 1 we plot the numerical solution for several time levels computed using a uniform mesh and with $\Delta t = 10^{-4}$.

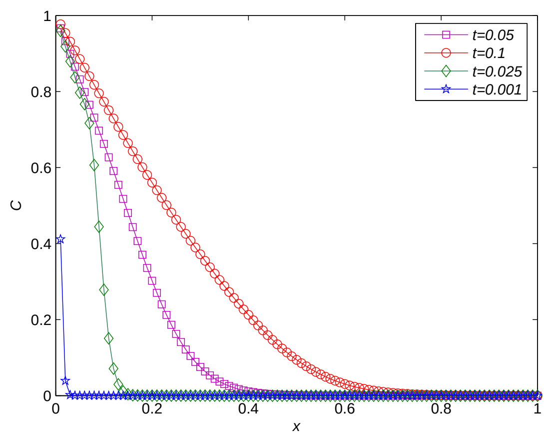

FIGURE 1. Numerical solution of (1) with the coefficients (62) and with the conditions (63).

In Table 1 we illustrate the convergence order established in Corollary 1. In this table we present the convergence rates given by

$$rate = \frac{\ln\left(\frac{\|P_{h_1}e_{h_1}\|_1}{\|P_{h_2}e_{h_2}\|_1}\right)}{\ln\left(\frac{h_1}{h_2}\right)}$$

where h_1 *and* $h_2 = \dfrac{h_1}{2}$ *are consecutive step-sizes that are contained in the first column of this table.*

Example 2. *Let us consider the equation (1) with* $\Omega = (0,1)$,

$$\begin{aligned} &a_2(x) = x+1,\ a_1(x) = x+1, a_0(x) = 0, \\ &b_2(x,t,s) = e^{-\frac{t-s}{\tau}}, b_1(s,t,x) = b_0(s,t,x) = 0, \end{aligned} \tag{64}$$

h	N	*error*	*rate*
1.000e-02	1.000e+02	3.796e-06	2.00
5.000e-03	2.000e+02	9.484e-07	2.00
2.500e-03	4.000e+02	2.370e-07	2.00
1.250e-03	8.000e+02	5.916e-08	2.01
6.250e-04	1.600e+03	1.470e-08	2.03
3.125e-04	3.200e+03	3.590e-09	2.13
1.563e-04	6.400e+03	8.188e-10	-

TABLE 1. Convergence rates for (1) with the coefficients (62) and with the conditions (63).

and $\tau = 0.01, T = 0.1$. *The reaction term* f *and the initial condition* u_0 *are such that the IVBP defined with (1) has the solution* $u(x,t) = tx(x-1)\cos(x)$.

We consider a set of 451 *random grids in* $[0,1]$ *and for the time integration we take* $\Delta t = 2 \times 10^{-6}$. *We plot in Figure 2 the logarithm of the error* $\|P_h e_h\|_1$ *versus the logarithm of the maximum step-size. The straight line plotted in this figure is the least-squares fit to the points* $(\ln(h_{max}), \ln(\|P_h e_h\|_1))$. *As the slop of this straight line is* 2.0107, *the numerical results obtained confirm the estimate given in Corollary 1.*

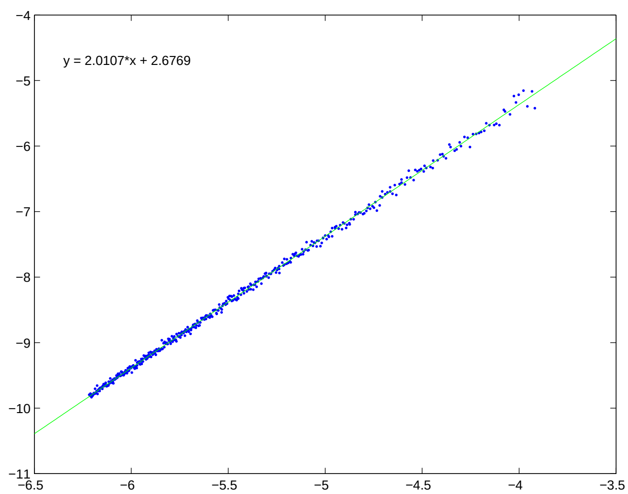

FIGURE 2. $\ln(\|P_h e_h\|_1)$ versus $\ln(h_{max})$.

Example 3. *Let us consider the equation (1) with* $\Omega = (0,1)$,

$$\begin{aligned} &a_2 = a_1 = 1, a_0 = 0, \\ &b_2(s,t,x) = e^{x - \frac{t-s}{\tau}} \sin(x), b_1(s,t,x) = e^{-\frac{t-s}{\tau}} x^2, b_0(s,t,x) = 0, \end{aligned} \tag{65}$$

and $\tau = 0.01$, $T = 0.1$. *Let* f *and* u_0 *be such that the IBVP defined with (1) has the solution* $u(t,x) = tx(x-1)\cos(x)$.

In Figure 3 we plot the logarithm of the error $\|P_h e_h\|_1$ *versus the logarithm of the maximum step-size for a set of* 451 *random grids considered in* $[0,1]$, *when* $\Delta t = 2 \times 10^{-6}$. *The least-squares straight line fitting the points* $(\ln(h_{max}), \ln(\|P_h e_h\|_1))$ *is also plotted in this figure. As the slop of this straight line is* 1.998 *we conclude that these results illustrate the estimates given in Corollary 1 .*

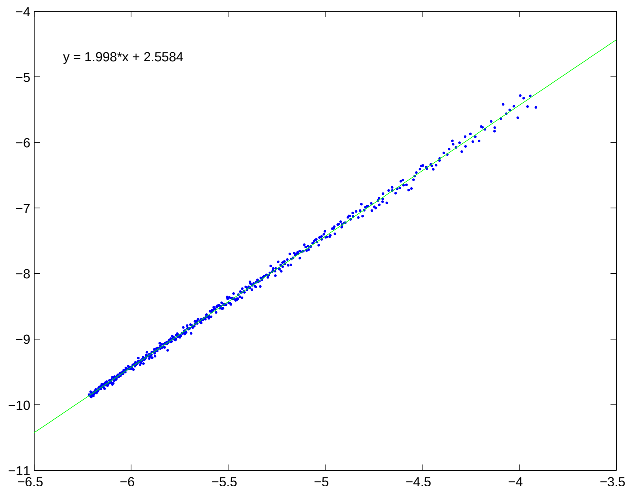

FIGURE 3. $\ln(\|P_h e_h\|_1)$ versus $\ln(h_{max})$.

6. Conclusions

In this paper a semi-discretization of the integro-differential problem (1) with Dirichlet boundary conditions was studied. It was shown that the semi-discrete approximation presents convergence of order r with respect to the norm $\|.\|_1$ provided that $u(t)$ and $\dfrac{\partial u}{\partial t}(t)$ are in $H^{r+1}(a,b)$ for $r \in \{1,2\}$. The semi-discretization studied can be seen as a standard finite difference discretization and as a lumped mass semi-discretization, and so the convergence estimates established can be seen as both supraconvergent and supercloseness estimates ([33]).

It is known that the semi-discrete approximation for the Fickian parabolic problem correspondent to (1), defined using the piecewise linear finite element method has second convergence order with respect to the L^2-norm provided the solution is in $H^2(a,b)$ ([32]). The smoothness required in the present paper is essential to conclude the unexpected convergence order obtained because the convergence was established considering the norm $\|.\|_1$.

7. Acknowledgements

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